Written exam of Condensed Matter Physics - September 9th 2022
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Exercise 1: Phonons.

Consider a one-dimensional crystal with chemical formula AB, composed of N unit cells, with lattice spacing a, hosting a two-atom basis. The atoms are constrained to move along the line that defines the crystal. The masses of the two inequivalent atoms are $M_{\rm A} = m$ and $M_{\rm B} = \frac{8}{7}m$, and K is the spring constant that describes the elastic force between nearest-neighbor atoms (see Fig. 1). Indicate with a_n and b_n the displacements of the two inequivalent atoms (respectively A and B) in the n-th unit cell, with respect to their equilibrium positions. Adopt periodic boundary conditions.

1. [5 points] Assuming traveling-wave solutions $a_n = \mathcal{A}{\rm e}^{i(qna-\omega t)}$ and $b_n = \mathcal{B}{\rm e}^{i(qna-\omega t)}$, where q is the one-dimensional wave vector, determine the dispersion of the acoustic and optical phonon branches, $\omega_a(q)$ and $\omega_o(q)$.

2. [4 points] Verify that, for small q, $\omega_a(q) \approx c_s|q|$, and determine the expression of the sound velocity c_s and of the minimum of the optical branch $(\omega_o)_{\min} \equiv \min_q \omega_o(q)$, as functions of K, a, and m.

3. [6 points] Let now $a = 0.231\,{\rm nm}$, $m = 2.32 \times 10^{-26}\,{\rm kg}$, and $K = 7.75\,{\rm kg/s^2}$. Determine the numerical value of the sound velocity c_s and of $(\omega_o)_{\min}$, then adopt a Debye model for the acoustic branch, $\omega_a(q) = c_s|q|$, and an Einstein model for the optical branch, with Einstein frequency $\omega_E = (\omega_o)_{\min}$, to calculate the specific heat c_V of the lattice at very high temperatures ($\kappa_B T \gg \hbar\omega_E$), and at $T = 1\,{\rm K}$. Note that $\int_0^\infty \frac{x}{{\rm e}^x-1}\,{\rm d}x = \frac{\pi^2}{6}$.

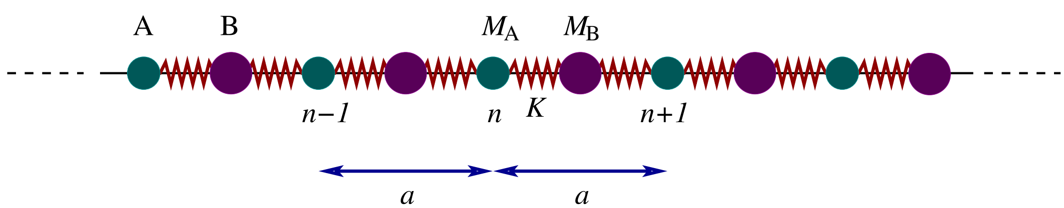

Fig. 1.

Exercise 2: Semiconductors.

In an n-type semiconductor (namely, doped with donors having concentration $N_d = 10^{20}\,{\rm m^{-3}}$) the conduction and valence bands can be approximated close to the band gap energy by the following relationships

$$E_C = E_g + Aa^2(k_x^2 + k_y^2 + k_z^2),$$
$$E_V = -Ba^2(k_x^2 + k_y^2 + k_z^2),$$

respectively, where E_g is the band gap, $A = 2.0\,{\rm eV}$, $B = 0.5\,{\rm eV}$ and $a = 0.3\,{\rm nm}$. At $T = 500\,{\rm K}$ the semiconductor is in an intrinsic regime, with carrier concentration equal to $1.4 \times 10^{22}\,{\rm m^{-3}}$.

1. [6 points] Determine the band gap energy at $T = 500\,{\rm K}$.

2. [5 points] Determine the sample electrical conductivity σ at $T = 500\,{\rm K}$, knowing that the electron and hole relaxation times are $\tau_e = 1.0 \times 10^{-12}\,{\rm s}$ and $\tau_h = 3.5 \times 10^{-12}\,{\rm s}$, respectively.

3. [4 points] Assuming that the carrier effective mass and relaxation time do not change with temperature, evaluate the sample electrical conductivity at $T = 10\,{\rm K}$, knowing that the carrier concentration at that temperature is $n_c = 2.6 \times 10^{18}\,{\rm m^{-3}}$ (extrinsic regime).

[Useful constants and conversion factors: the Planck constant is $\hbar = 1.05 \times 10^{-34}\,{\rm J\cdot s}$, the Boltzmann constant is $\kappa_B = 1.38 \times 10^{-23}\,{\rm J\cdot K^{-1}}$, the elementary charge is $e = 1.60 \times 10^{-19}\,{\rm C}$, the free electron mass is $m_0 = 9.11 \times 10^{-31}\,{\rm kg}$; $1\,{\rm eV}$ corresponds to a temperature of $1.16 \times 10^4\,{\rm K}$ or to an energy of $1.60 \times 10^{-19}\,{\rm J}$].

Solution
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Exercise 1.

1. The equations of motion are

$$\begin{cases} M_\mathrm{A}\ddot{a}_n = -K\left(2a_n - b_n - b_{n-1}\right), \\ M_\mathrm{B}\ddot{b}_n = -K\left(2b_n - a_{n+1} - a_n\right). \end{cases}$$

Substituting the traveling-wave solutions, we find

$$\begin{cases} \left(2K - M_\mathrm{A}\omega^2\right)\mathcal{A} - K\left(1+\mathrm{e}^{-iqa}\right)\mathcal{B} = 0, \\ -K\left(1+\mathrm{e}^{iqa}\right)\mathcal{A} + \left(2K - M_\mathrm{B}\omega^2\right)\mathcal{B} = 0, \end{cases}$$

which admits nontrivial solutions for $\mathcal{A},\mathcal{B}$ if and only if the determinant of the matrix associated to the system of linear equations vanishes. Letting in the following $\overline{\Omega} \equiv \sqrt{K(M_\mathrm{A}+M_\mathrm{B})/(M_\mathrm{A}M_\mathrm{B})} = \sqrt{\frac{15K}{8m}}$, which is the relevant frequency scale in our problem, the equation that determines the phonon frequencies reads

$$\omega^4 - 2\overline{\Omega}^2\omega^2 + \frac{224}{225}\overline{\Omega}^4\sin^2\frac{qa}{2} = 0,$$

whose solutions are

$$\omega_\pm^2(q) = \overline{\Omega}^2\left(1 \pm \sqrt{1 - \frac{224}{225}\sin^2\frac{qa}{2}}\right),$$

with $\omega_a(q) = \omega_-(q)$ and $\omega_o(q) = \omega_+(q)$ describing the acoustic and optical phonon branch, respectively.

2. For the acoustic branch, since for $|q|a \ll 1$ we have $\sin^2\frac{qa}{2} \approx \left(\frac{qa}{2}\right)^2$ and $\sqrt{1 - \frac{56}{225}(qa)^2} \approx 1 - \frac{28}{225}(qa)^2$, we find

$$\omega_a(q) \approx c_s|q|, \qquad \text{with } c_s = \frac{2\sqrt{7}}{15}\overline{\Omega}a = \sqrt{\frac{7K}{30m}}\,a.$$

The minimum of the optical branch is found at $q = \frac{\pi}{a}$, and is $(\omega_o)_\mathrm{min} = 4\overline{\Omega}/\sqrt{15} = \sqrt{2K/m}$.

3. Inserting the values given in the text, we find

$$c_s = 2.04\times10^3\ \mathrm{m/s}; \qquad (\omega_o)_\mathrm{min} = 2.58\times10^{13}\ \mathrm{s}^{-1}.$$

As suggested by the text, we set $\omega_E = (\omega_o)_\mathrm{min}$. Then, the internal energy per unit volume is

$$u = \sum_{s=a,o}\int_{-\pi/a}^{\pi/a}\frac{\mathrm{d}q}{2\pi}\frac{\hbar\omega_s(q)}{\mathrm{e}^{\beta\hbar\omega_s(q)}-1} \approx \int_0^{q_D}\frac{\mathrm{d}q}{\pi}\frac{\hbar c_s q}{\mathrm{e}^{\beta\hbar c_s q}-1} + \frac{1}{a}\frac{\hbar\omega_E}{\mathrm{e}^{\beta\hbar\omega_E}-1},$$

with $\beta = 1/(k_BT)$, and $q_D = \pi/a$, because in one dimension the Debye sphere coincides with the first Brillouin zone.

At high temperature, $k_BT \gg \hbar\omega_D, \hbar\omega_E$, with $\omega_D \equiv c_s q_D$, the exponentials in the denominators can be expanded to first order, the two phonon modes give the same contribution (equipartition), and

$$u \approx \frac{2k_BT}{a} \quad \Rightarrow \quad c_V = \frac{2k_B}{a} \equiv c_V^{DP},$$

i.e., we recover the Dulong-Petit (DP) value for a one-dimensional crystal with two atoms per unit cell. For the given set of parameters $c_V \approx 1.195\times10^{-13}$ J/(K·m).

At low temperature, $k_BT \ll \hbar\omega_D, \hbar\omega_E$,

$$u \approx \frac{\hbar c_s}{\pi}\left(\frac{k_BT}{\hbar c_s}\right)^2\int_0^\infty\frac{x}{\mathrm{e}^x-1}\,\mathrm{d}x + \frac{\hbar\omega_E}{a}\mathrm{e}^{-\beta\hbar\omega_E} \approx \frac{\pi^2\hbar\omega_D}{6a}\left(\frac{k_BT}{\hbar\omega_D}\right)^2 \quad \Rightarrow \quad c_V = \frac{\pi^2k_B}{3a}\left(\frac{k_BT}{\hbar\omega_D}\right),$$

where we adopted the change of variable $x = \beta\hbar c_s q$ in the integral over q, and extended the integration limit to infinity, to extract the leading behavior at small T. In the final expression for u, we neglected the exponentially small contribution of the optical branch, since the numerical estimate gives $\Theta_E \equiv \hbar\omega_E/k_B = 197\,\mathrm{K}$, i.e., at $T = 1\,\mathrm{K}$, $\mathrm{e}^{-\beta\hbar\omega_E} \approx \mathrm{e}^{-197} \approx 2.78 \times 10^{-86}$. Thus, at $T = 1\,\mathrm{K}$, $c_V \approx 0.0155\,k_B/a \approx 7.76 \times 10^{-3}\,c_V^{DP} = 9.27 \times 10^{-16}\,\mathrm{J/(K{\cdot}m)}$, where we used the numerical value of the Debye temperature $\Theta_D \equiv \hbar\omega_D/k_B = 212\,\mathrm{K}$.

Exercise 2.

1. Given the carrier concentration in the intrinsic regime:

$$n_c = p_v = n_i = 2.5 \cdot (0.212 \cdot 0.847)^{3/4} \left(\frac{5}{3}\right)^{3/2} \cdot \mathrm{e}^{-E_g/(2\cdot 0.043)} \times 10^{25}\,\mathrm{m}^{-3} = 1.40 \times 10^{22}\,\mathrm{m}^{-3},$$

where the electron and hole effective mass used are $m_e = \hbar^2/(2Aa^2) = 1.928 \times 10^{-31}\,\mathrm{kg} = 0.212\,m_0$ and $m_h = \hbar^2/(2Ba^2) = 7.713 \times 10^{-31}\,\mathrm{kg} = 0.847\,m_0$, respectively, one finds $E_g = 0.60\,\mathrm{eV}$.

2. The electrical conductivity at $T = 500\,\mathrm{K}$ is given by

$$\sigma = n_i e^2 \left(\frac{\tau_e}{m_e} + \frac{\tau_h}{m_h}\right) = 3.5 \times 10^3\,\Omega^{-1} \cdot \mathrm{m}^{-1}.$$

3. At $T = 10\,\mathrm{K}$ only electrons ionized from the donors contribute to the electrical conductivity, thus

$$\sigma = n_c e^2 \frac{\tau_e}{m_e} = 3.5 \times 10^{-1}\,\Omega^{-1} \cdot \mathrm{m}^{-1}.$$